

# High field transport in strained Si/GeSi double heterostructure: a Fokker-Planck approach

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We report calculations of high electric field transport for the case of a strained Si/GeSi double heterostructure (DHS) considering transport along the Si channel and by applying the analytical Fokker-Planck approach (FPA), where the process is modeled as drift-diffusion in energy space. We limit ourselves to electronic transport in the conduction band of the strained Si, where an energy shift between the otherwise degenerate six energy valleys characterizes the band alignment in the DHS. Intervalley phonon scatterings are considered while intravalley acoustic phonon scattering is ignored, leading to results valid for high enough temperatures. Our results are compared to previous theoretical works where Monte Carlo simulations were applied. A reasonable agreement between the two approaches is obtained in the high electric field regime.

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## I. INTRODUCTION

Important developments have been taking place in the growth of strained heterostructures based on Si and  $\text{Ge}_x\text{Si}_{1-x}$  layers [1,2]. The particular case of Si layers pseudomorphically grown on relaxed  $\text{Ge}_x\text{Si}_{1-x}$  buffers is rather interesting because of the large mobilities reported, exceeding the corresponding bulk Si values [3,4]. It has been shown that in this type of double heterostructures (DHS) the otherwise degenerate six  $\Delta_6$  valleys of bulk Si are shifted in energy. If the DHS is grown along a high symmetry direction (say, the  $\langle 001 \rangle$  direction), the two valleys along this direction are shifted downwards in energy, while the other four valleys are shifted upwards. As a result, we are led to two  $\Delta_2$  valleys with a bottom energy below the corresponding one for the bulk valleys and four  $\Delta_4$  valleys with a higher bottom energy. The energy shift between the  $\Delta_2$  and  $\Delta_4$  valleys is empirically estimated as  $\Delta E = 0.6x$  eV. In this kind of DHS, a quantum-well like band alignment in the Si channel was unexpectedly found in 1985 [1,2], which is due to tensile strains in Si and ensures high-mobility  $n$  channel for the doped structure. High mobilities are explained as a consequence of the low effective mass of the carriers in  $\Delta_2$  valleys and also because the scattering efficiency of the carriers (by phonons and impurities) is reduced. The above mentioned facts are of great importance for device performance and this kind of structures seems to have a prominent future for applications in micro and optoelectronics [2].

Monte Carlo calculations of high electric field mobilities and drift velocities for electronic transport along the Si channel of  $\text{Si}/\text{Ge}_x\text{Si}_{1-x}$  were reported by various authors [5–8] and also applied in the study of modulation-doped field-effect transistor (MODFET) structures [9]. More recently, hole transport parameters have been analyzed for this type of systems [10]. While the electronic transport properties of low field, low temperature  $\text{Si}/\text{GeSi}$  heterostructures are more or less well understood [11], the situation is not the same for high electric fields. For high field transport, the effects of size quantization are usually negligible and we can work within three dimensional models for the valley structure. In Ref. [7], size quantization was introduced in a 10 nm Si channel, but the authors had to include up to six subbands in the  $\Delta_2$  valleys. Strain effects are introduced through the splitting energy  $\Delta E$  between the  $\Delta_2$  and  $\Delta_4$  valleys, which ranges from 0.1 eV to 0.4 eV. Such relatively large values of the energy shift effectively reduce the intervalley phonon scatterings between the valleys (in comparison with the unstrained Si).

In the present paper we report results for high electric field electronic transport along the Si channel of a  $\text{Si}/\text{GeSi}$  DHS. We model the system in close analogy with the above mentioned works, taking into account the energy shift between the  $\Delta_2$  and  $\Delta_4$  valleys and neglecting size quantization. Rather than Monte Carlo simulations, we apply an analytical Fokker-Planck approach (FPA), which treats transport as an energy-diffusion process in energy space. This approach was proposed a long time ago [12,13] as an alternative for the consideration of high-field transport in semiconductors. The theory bears a semiclassical nature and has been recently revisited, the general formalism being discussed with further details [14–16]. As a test of the FPA in the case of a well known semiconductor, the present authors applied the theory to bulk Si, where both experimental data and Monte Carlo simulations for the high field drift velocity were successfully reproduced [17]. The current calculations can also be considered as a way of testing the FPA in a somewhat different system, which is of present day interest in high technology applications.

The FPA is applicable when the energy exchanges between the carriers and the surrounding medium (crystal lattice + external field) can be assumed quasicontinuous. This latter condition apparently invalidates the method for highly inelastic scattering mechanisms (as is the case of carrier scattering by optic and intervalley phonons). However, if the carrier energy is large enough, the exchanged energy becomes certainly low compared with the energy of the carriers, and this is the case of high field transport. Hence, the FPA is assumed to be valid if the condition  $E_{av} \gg \hbar\omega$  is fulfilled, where  $E_{av}$  is the average carrier energy and  $\hbar\omega$  the exchanged energy (say, the phonon energy). The FPA has the advantage of being analytical, and, whenever it can be applied, saves computational time and allows a more transparent physical interpretation. Of course, it cannot compete in accuracy with Monte Carlo simulations. However, we have found that the FPA leads to comparatively good results even in cases where several scattering mechanisms should be taken into account [17]. In contrast with Monte Carlo simulations, the analytical approach involves less realistic models for the analysis of a concrete semiconductor. More details about the applied model and the fundamental theory are given in the next sections.

The paper is organized as follows. In Sec. II we briefly summarize general theoretical aspects of our work, in Sec. III details of the calculations for the  $\text{Si}/\text{GeSi}$  DHS are presented, in Sec. IV the results of our calculations are shown and comparison with previous works is made.

## II. GENERAL THEORY

The FPA considers transport in the spirit of a drift-diffusion process in energy space. A certain distribution function (DF),  $f(E, t)$ , is defined which depends on the carrier energy  $E$  and the time  $t$ , such that  $f(E, t)N(E)$  gives the number

of carriers at time  $t$  having their energies in the interval  $[E, E + dE]$ , while the function  $N(E)$  represents the density of states (DOS). The DF obeys the equation [12–16] :

$$\frac{\partial}{\partial t} f(E, t) + \frac{1}{N(E)} \frac{\partial}{\partial E} J(E, t) = 0, \quad (1)$$

where

$$J(E, t) = W(E)N(E)f(E, t) - \frac{\partial}{\partial E} [D(E)N(E)f(E, t)]. \quad (2)$$

In Eq. (2)  $W(E)$  represents a certain “drift velocity” of the carriers in energy space and in fact gives the rate of energy exchange of the carriers with the surrounding medium, while  $D(E)$  is a kind of diffusion coefficient. Equation (1) has the form of a continuity equation for the carrier “motion” in energy space and leads to the conservation of the carrier “flux”. For a many valley system it should be applied to each of the valleys separately and it is worth to note that Eq. (1) does not describe intervalley couplings. The quantity  $J(E, t)$ , given by Eq. (2), is thus the carrier current density in energy space. Under steady-state conditions the DF is time independent. Moreover, we must have  $J(E) = 0$ . Hence, we are led to

$$\frac{\partial}{\partial E} [D(E)N(E)f(E)] = W(E)N(E)f(E). \quad (3)$$

We assume the existence of a phonon bath in equilibrium at the temperature  $T$ . The carriers interact with the phonons and the applied dc electric field  $\vec{F}$ . We suppose, as an approximation, that the continuous exchange of phonons between the carriers and the phonon bath does not affect the thermal equilibrium of the latter. The coefficients  $W(E)$  and  $D(E)$  are split as follows

$$D(E) = D_F(E) + D_{ph}(E) \quad , \quad W(E) = W_F(E) + W_{ph}(E). \quad (4)$$

The label “ $F$ ” (“ $ph$ ”) denotes the electric field (phonon) contribution to these coefficients. We are obviously neglecting the intracollisional field effect. The explicit form of these coefficients is obtained below.

Equation (3) has the simple solution

$$f(E) = \exp \left\{ \int \left[ \frac{W_{ph}(E)}{D_F(E)} dE \right] \right\}, \quad (5)$$

where  $D_{ph}(E)$  was neglected. This approximation is very well fulfilled in all the cases of interest for us [13,14]. The practical usefulness of the FPA lies in the possibility of the *analytical* performance of the integral in Eq. (5).

Let us apply the above formalism to electrons in the  $\Delta_2$  energy valleys of strained Si of a Si/Ge<sub>x</sub>Si<sub>1-x</sub> DHS. The  $\Delta_2$  valleys are ellipsoids of revolution in  $\vec{k}$ -space with their revolution axis along the  $\langle 001 \rangle$  crystallographic direction, coincident with the growth direction of the DHS. To be specific, let us take  $\vec{F} = (0, F, 0)$ , where the  $x, y, z$  coordinates are taken along  $\langle 100 \rangle$ ,  $\langle 010 \rangle$  and  $\langle 001 \rangle$  respectively. The energy dispersion relation is given in the form  $\epsilon = \epsilon(\vec{p})$ . In order to take into account non-parabolicity of the band structure, we assume

$$\gamma(\epsilon) = \epsilon(1 + \alpha\epsilon) = \frac{p_t^2}{2m_t} + \frac{p_l^2}{2m_l} = \frac{p^{*2}}{2m_0}. \quad (6)$$

In Eq. (6)  $m_t$  ( $m_l$ ) is the transverse (longitudinal) effective mass of the bulk Si conduction band electrons. We suppose the masses are not changed by the strains in the Si layer:  $m_t/m_0 = 0.19$  and  $m_l/m_0 = 0.916$ . Nonparabolicity is estimated also the same as in bulk Si:  $\alpha = 0.5$  (eV)<sup>-1</sup>. The Herring-Vogt transformation was applied in writing the right-hand side (RHS) of Eq. (6), where  $p_t = (m_t/m_0)^{1/2} p_t^*$ ,  $p_l = (m_l/m_0)^{1/2} p_l^*$  and  $p^{*2} = p_t^{*2} + p_l^{*2}$ .

The explicit expressions for  $D_F(E)$  and  $W_{ph}(E)$  can be directly taken from Refs. [13–15]. Hence, for  $D_F(E)$  we have

$$D_F(E) = \frac{2e^2 F^2}{3m_t} \tau(\epsilon) \gamma(\epsilon) / (\gamma'(\epsilon))^2, \quad (7)$$

where  $\gamma'(\epsilon)$  denotes the first derivative of the function (defined in Eq. (6)). For  $\tau(\epsilon)$  we shall consider one “ $g$ ” intervalley phonon responsible for transitions between the equivalent  $\Delta_2$  valleys. Then the relaxation time reads as

$$\frac{1}{\tau_g(\epsilon)} = C_g \left[ n_g(T) \sqrt{\gamma(\epsilon + \hbar\omega_g)} |1 + 2\alpha(\epsilon + \hbar\omega_g)| \right]$$

$$+(n_g(T) + 1)\sqrt{\gamma(\epsilon - \hbar\omega_g)}|1 + 2\alpha(\epsilon - \hbar\omega_g)\theta(\epsilon - \hbar\omega_g)|\Big], \quad (8)$$

where  $\theta(\epsilon)$  is the step-function,

$$n_g(T) = [\exp(\hbar\omega_g/k_B T) - 1]^{-1}, \quad (9)$$

and

$$C_g = \frac{m_d^{3/2} D_g^2}{\sqrt{2}\pi\rho\hbar^3\omega_g}. \quad (10)$$

In Eq. (10)  $\rho$  is the semiconductor mass density,  $\omega_g$  and  $D_g$  are the phonon frequency and deformation-potential (DP) constant respectively for intervalley phonons of type “ $g$ ”. As a simplified model for our calculations, we have considered just one “ $g$ ” phonon with an energy  $\hbar\omega_g = 0.031$  eV and DP coupling constant  $D_g = 11 \times 10^8$  eV/cm, which approximately corresponds to the average of the three “ $g$ ” phonons of bulk Si reported in Table VI of Ref. [18]. Other bulk Si parameters are also taken from the same reference.

For ellipsoidal  $\Delta_2$ -valleys of the Si layer CB, the DOS is given by

$$N(E) = \frac{V m_d^{3/2}}{\sqrt{2}\pi^2 \hbar^3} \sqrt{E(1 + \alpha E)} |1 + 2\alpha E|, \quad (11)$$

where nonparabolicity is taken into account and  $m_d = \sqrt[3]{m_t^2 m_L}$ . In calculating  $W_{ph}(E)$ , we use the expression

$$W_{ph}(E) = \hbar\omega [1/\tau_{abs}(\vec{p}) - 1/\tau_{em}(\vec{p})], \quad (12)$$

where “ $abs$ ” (“ $em$ ”) denotes phonon absorption (emission) by the electron. We must remember that

$$1/\tau(\epsilon) = 1/\tau_{abs}(\epsilon) + 1/\tau_{em}(\epsilon), \quad (13)$$

the “ $abs$ ” (“ $em$ ”) term in Eq. (13) corresponds to the first (second) term at the RHS of Eq. (8) for the case of intervalley “ $g$ ” phonons. Hence, using Eq. (12) and latter expressions for  $\tau_{abs}$  and  $\tau_{em}$ , we can find the explicit form of  $W_{ph}^g$ .

Intravalley optical phonons do not contribute to transition rates because the corresponding transitions are forbidden by the selection rules. The contribution of intravalley acoustic phonons will be ignored in the present work. For high temperatures and high carrier energies they should provide a weak contribution to transport parameters and we shall limit ourselves to this case.

As was remarked above, intervalley phonon scattering, strictly speaking, is beyond the scope of the Fokker-Planck equation in its standard form [Eq. (1)]. After the absorption or the emission of an intervalley phonon, the electron is dropped away from one valley into another one, and such abrupt transitions are not explicitly assumed in Eq. (1), where the electron number is conserved within each valley. However, when we have equivalent valleys (as is the case of  $\Delta_2$  valleys), we can still apply the Fokker-Planck equation in its standard form; electrons dropped away from one valley fall into an equivalent one and vice versa, all happens as the electrons always remained within the given valley. Of course, if the valleys are not equivalent this argument no longer applies. This is the case of electron transitions induced by the “ $f$ ” intervalley phonons between valleys  $\Delta_2$  and  $\Delta_4$ , which are not equivalent in the strained Si layer of the Si/GeSi DHS. For such intervalley electronic transitions we must consider a different approach.

In order to estimate the effect of electron intervalley transitions due to the interaction with “ $f$ ” intervalley phonons we must realize that this effect is actually weak and should introduce just small changes into our final results. As for the case of “ $g$ ” intervalley phonons, we assume just one type of “ $f$ ” phonons with energy  $\hbar\omega_f = 0.042$  eV and DP coupling constant  $D_f = 4 \times 10^8$  eV/cm (we again estimated these parameters as averages from the three corresponding “ $f$ ” phonons reported in Table VI of Ref. [18]). In all cases we considered zero-order intervalley phonons in our model (a more realistic model must consider first order intervalley phonons in the way discussed in Ref. [19]). Electron transitions due to the interaction with “ $f$ ” intervalley phonons from  $\Delta_2$  valleys up to  $\Delta_4$  valleys is formally switched on at  $t = 0$  and the DF in each of the  $\Delta_2$  valleys evolves in time by the approximate law  $\frac{df}{dt} = -f/\tau_f$ , where  $\tau_f$  and the corresponding expressions for  $n_f(T)$  and  $C_f$  are obtained from Eqs.(8), (9) and (10) by means of the formal substitution:  $g \rightarrow f$  and  $\epsilon \rightarrow \epsilon - \Delta E$ .

After a time  $\tau$  has elapsed, we obtain the result

$$f(E, \tau) = f(E) \exp[-\tau/\tau_f(E)], \quad (14)$$

where  $f(E)$  represents the DF without taking the  $\Delta_2$ - $\Delta_4$  intervalley scattering into account. Of course, this is just a rough estimation of the effect and we are actually neglecting the inverse intervalley process (from  $\Delta_4$  to  $\Delta_2$  valleys). Due to the weakness of the effect, we shall assume that this procedure is satisfactory. For the parameter  $\tau$  in Eq. (14), we make the reasonable estimate

$$\tau = \frac{1}{eF} \left[ \frac{m_t \hbar \omega_f}{2n_f(T) + 1} \right]^{1/2}. \quad (15)$$

### III. CALCULATION OF THE DISTRIBUTION FUNCTION

From Eq. (5), with the explicit application of Eqs. (7) and (12), we are led to the DF for  $\Delta_2$  valleys without the consideration of the  $\Delta_2$ - $\Delta_4$  intervalley scattering process. The final result is

$$f_j(E) = E^{A_j} (1 + \alpha E)^{B_j} \exp(\beta_t E P_j(E, T)), \quad j = 1, 2, \quad (16)$$

where  $A_j$  and  $B_j$  are parameters (dependent on  $T$  and  $F$ ) and  $P_j(E, T)$  is a polynomial in  $E$ . This structure is far from the Maxwellian one. The DF describes a stationary non-equilibrium configuration where an electron temperature  $T_e$  cannot be defined. In Eq. (16) we shall measure all energies in units of  $\hbar\omega_g$  and

$$\beta_t = \frac{3m_t m_d^3 D_g^4}{4\pi^2 \rho^2 \hbar^4 e^2 F^2}. \quad (17)$$

For  $E < 1$  we obtain

$$\begin{aligned} A_1 &= \beta_t (n_g(T))^2 (1 + E_0)(1 + 2E_0)^2 \\ B_1 &= \beta_t (n_g(T))^2 (E_0 - 1)(E_0 - 1/2)^2 \\ P_1(E, T) &= (n_g(T))^2 \sum_{i=0}^4 a_{i1} E^i, \end{aligned} \quad (18)$$

where the  $a_{i1}$  are coefficients explicitly dependent on  $E_0 = \hbar\omega_g\alpha$ . For  $E > 1$  the following result is obtained

$$\begin{aligned} A_2 &= \beta_t [(n_g(T))^2 2(1 + 8E_0^2) - (2n_g(T) + 1)(4E_0^3 - 8E_0^2 + 5E_0 - 1)] \\ B_2 &= \beta_t [(n_g(T))^2 2(8E_0^2 + 1) + (2n_g(T) + 1)(4E_0^3 + 8E_0^2 + 5E_0 + 1)] \\ P_2(E, T) &= \sum_{i=0}^4 a_{i2} E^i, \end{aligned} \quad (19)$$

where the coefficients  $a_{i2}$  are now dependent on  $T$  through  $n_g(T)$ . All the coefficients  $a_{ij}$  are given in Table I.

In the interval  $E > 1$  we must distinguish three subintervals:  $1 < E < \Delta E - E_f$ ,  $\Delta E - E_f < E < \Delta E + E_f$  and  $E > \Delta E + E_f$ , where  $E_f = \hbar\omega_f/\hbar\omega_g$ . In the latter two subintervals, the DF shall be given by

$$f_j(E, \tau) = f_2(E) \exp[-\tau/\tau_f(E)] \quad , \quad j = 3, 4, \quad (20)$$

in correspondence with our approach to intervalley transitions between  $\Delta_2$  and  $\Delta_4$  valleys.

Once we have determined the DF, we can calculate the electron average energy by the expression

$$E_{av} = \int \{E f(E) N(E)\} dE / \int \{f(E) N(E)\} dE. \quad (21)$$

In Eq. (21) we just consider  $\Delta_2$  valleys, i.e., we assume the  $\Delta_4$  valleys essentially deprived of carriers, an approximation that seems acceptable if the applied electric field is not extremely large. Moreover, in Eq. (21) we should be careful in partitioning the integration into the four energy subintervals mentioned above.

Another important quantity is the drift velocity  $v_d$  given by

$$v_d = \frac{2eF}{3m_t} \int \left\{ \frac{\gamma(E)\tau_g(E)}{(\gamma'(E))^2} \left[ -\frac{df}{dE} \right] N(E) \right\} dE / \int \{f(E) N(E)\} dE. \quad (22)$$

In Eq. (22) we must partition the integration in the same way as in Eq. (21). We just considered the drift velocity from electrons in the  $\Delta_2$  valleys.

## IV. DISCUSSION OF RESULTS

By direct application of the theory developed in the foregoing sections, we have made numerical calculations of the average electron energy  $E_{av}$  and the electron drift velocity  $v_d$  as functions of the temperature  $T$  and dc electric field  $F$ . Our results are essentially valid for high temperatures as far as intravalley acoustic phonon scattering was ignored. As it was remarked in Sec. I, the FPA is applicable for high electric fields, when the condition  $E_{av} \gg \hbar\omega$  fulfils [14,15]. In the examined Si/GeSi DHS, we take into account the relatively large energy shift between valleys  $\Delta_2$  and  $\Delta_4$  and consider that just the  $\Delta_2$  valley is substantially populated by carriers. Hence, intervalley transitions between valleys  $\Delta_2$ - $\Delta_4$  are assumed to be weak processes and treated within a relatively coarse approximation. As it was discussed in the previous sections, such transitions are actually beyond the scope of standard FPA. All numerical parameters used in computations were taken from Ref. [18] and also shown in Sec. III.

In Fig. 1 we show our results for the average electron energy  $E_{av}$  as a function of electric field  $F$  for  $T = 300$  K. Two values of  $\Delta E$  were considered: 0.4 and 0.1 eV. As expected, the results show a rather weak dependence on  $\Delta E$ . The involved carrier energies are large enough, thus ensuring the applicability of the FPA. After comparison of Fig. 1 with Fig. 1(a) of Ref. [5], we can see that a reasonable agreement was actually achieved. It is important to notice that just one fitting parameter was applied in the  $\beta_t$  of Eq. (17), which could be related to the overlapping integral describing the electron-phonon scattering probabilities. This overlapping integral was assumed unity in the general formulas of Sec. II, but actually it differs from unity when intervalley phonons are present. The linear behavior of  $E_{av}$  for  $F \lesssim 5$  kV/cm should not be realistic because the FPA is not valid in the low-field regime as discussed exhaustively in previous works. [14–16]

In Fig. 2 we present the drift velocity  $v_d$  as a function of the electric field for  $T = 300$  K. The continuous curve represents our calculations, while the dots were taken from Fig. 2(a) of Ref. [15]. We just considered the case  $\Delta E = 0.2$  eV. As a matter of fact, the curves for different values of  $\Delta E$  are almost coincident (in close agreement with the results shown in Ref. [15]) as can be expected from general physical grounds. For lower electric fields our results deviate from those of Ref. [15], a reasonable result taking into account that the FPA is valid for high electric fields. However, for very high electric fields ( $F > 80$  kV/cm) we again notice an increasing deviation from the Monte Carlo results of Ref. [15]. The FPA is not able to describe the saturation value of  $v_d$  in the very high electric field region. On the contrary, it is obtained a decreasing behavior of the drift velocity at a rate that becomes much higher as higher is the field. In our present treatment (as well as in that of Ref. [15]) negative differential mobilities are out of question as far as the contributions of electrons from the  $\Delta_4$  valleys are not considered. As a final remark, we should notice a very good agreement with the results of Ref. [15] for a wide interval of electric fields.

In Fig. 3 we show the same plots as those of Fig. 2, but now for  $T = 77$  K. From a simple glance at Fig. 3, it is obvious that for such a low temperature the agreement between the FPA and the Monte Carlo results of Ref. [15] (Fig. 2(b)) is much worse. As it was discussed before, we have ignored intravalley acoustic phonons. Even though this is not a limitation of the FPA itself, it is a difficult task to include them in the calculations. Furthermore, at low temperatures, quantum effects should become relevant and a quantum approach should be required. Hence, we stress that the FPA results are reliable just for high temperatures.

In this work we have compared our results with those from Monte Carlo simulations. [15] Other possible comparisons could be done. For instance, we could compare with Fig. 3 of Ref. [8] or Ref. [6]. But all these results are in accordance with themselves and nothing essential would be added. Our results are also comparable to those of Ref. [7], where size quantization was examined. As it was said before, size quantization is of relevance when the carrier energies are low enough (this is the case of low field transport as discussed in Ref. [11]), but for the high carrier energies involved in high field transport, size quantization becomes irrelevant. In the revised literature we have not found available experimental data for this kind of system. As a general remark, we conclude that the FPA leads to results in acceptable agreement with those of Monte Carlo simulations in those intervals of temperature and electric fields where it is supposed to be valid. This conclusion is true in spite of the more or less coarse simplifications we have to face within the limits of this method. However, if wider intervals of electric fields or more accurate treatment is required, Monte Carlo simulations or some other equivalent numerical procedure should be necessary.

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## FIGURES

FIG. 1. Average electron energy ( in eV) as a function of the electric field for  $T = 300$  K. Two values of  $\Delta E$  are examined: 0.4 and 0.1 eV.

FIG. 2. Drift velocity as a function of the electric field for  $T = 300$  K. Our results are represented by the continuous while the dots were taken from Monte Carlo simulations of Ref. [15]. We have set  $\Delta E = 0.2$  eV.

FIG. 3. Same as in Fig. 2 for  $T = 77$  K. The dots are Monte Carlo results from Ref. [15]. As one can see the agreement is now much worse.

TABLE I. Coefficients  $a_{ij}$ :  $i = 0, \dots, 4$ ,  $j = 1, 2$

|   |   |
|---|---|
| $4E_0(4E_0^3 + 8E_0^2 + 11E_0 + 3) + 1$ | $8E_0(8E_0^2 + 3) + (2n_g + 1)(-16E_0^4 + 32E_0^3 - 44E_0^2 + 12E_0 - 1)$ |
| $4E_0(8E_0^3 + 12E_0^2 + 7E_0 + 1)$     | $8E_0^2 n_g^2 (8E_0^2 + 7) + (2n_g + 1)(8E_0^3 - 12E_0^2 + 7E_0 - 1)$     |
| $8E_0^2(2E_0 + 1)^2$                    | $64E_0^3 n_g^2 - 8E_0^2(2n_g + 1)(4E_0^2 - 4E_0 + 1)$                     |
| $8E_0^3(2E_0 + 1)$                      | $32E_0^4 n_g^2 + 8E_0^3(2n_g + 1)(2E_0 - 1)$                              |
| $16E_0^4/5$                             | $-16E_0^4(2n_g + 1)/5$  |







